

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
 Data File : BF141966.D
 Acq On : 14 Mar 2025 15:38
 Operator : RC/JU
 Sample : Q1545-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-02-031125

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	27	rVB	993012	1617326	55.61%	5.776%
2	5.493	571	578	583	rBV	1803489	2416529	83.09%	8.631%
3	6.492	742	748	762	rBV	1688412	2280224	78.40%	8.144%
4	6.875	808	813	820	rBV	627239	785567	27.01%	2.806%
5	7.434	899	908	913	rBV	1207877	1541482	53.00%	5.505%
6	7.687	946	951	960	rBV	47991	67241	2.31%	0.240%
7	8.157	1025	1031	1044	rBV	719618	956406	32.88%	3.416%
8	8.369	1062	1067	1075	rVB5	21203	36612	1.26%	0.131%
9	9.228	1208	1213	1223	rBV	2124050	2685211	92.33%	9.590%
10	9.310	1223	1227	1235	rVB2	20610	31450	1.08%	0.112%
11	9.633	1277	1282	1288	rBV3	20973	33421	1.15%	0.119%
12	9.769	1301	1305	1312	rBV	127841	168991	5.81%	0.604%
13	9.910	1323	1329	1334	rBV	685234	857523	29.48%	3.063%
14	10.622	1445	1450	1457	rBV	531854	664771	22.86%	2.374%
15	10.698	1457	1463	1475	rVV	1133938	1521193	52.30%	5.433%
16	10.822	1479	1484	1491	rVB3	30920	51758	1.78%	0.185%
17	10.933	1498	1503	1507	rVB	71223	90282	3.10%	0.322%
18	11.398	1576	1582	1589	rBV	621788	917659	31.55%	3.277%
19	11.469	1591	1594	1597	rVV	35648	50683	1.74%	0.181%
20	11.845	1654	1658	1662	rBV5	25297	44652	1.54%	0.159%
21	11.922	1664	1671	1677	rBV2	477158	684945	23.55%	2.446%
22	12.010	1682	1686	1694	rVB	61269	124232	4.27%	0.444%
23	12.092	1697	1700	1704	rBV4	21516	32387	1.11%	0.116%
24	12.445	1757	1760	1763	rVB	39689	43427	1.49%	0.155%
25	12.480	1764	1766	1771	rVB2	26066	34003	1.17%	0.121%
26	12.527	1771	1774	1779	rBV2	43878	62849	2.16%	0.224%
27	12.610	1783	1788	1793	rBV	400813	567025	19.50%	2.025%
28	12.704	1800	1804	1811	rBV	189468	282562	9.72%	1.009%
29	12.833	1821	1826	1832	rBV	473526	676803	23.27%	2.417%
30	12.980	1846	1851	1858	rVB	2284170	2908351	100.00%	10.387%
31	13.057	1860	1864	1871	rVV3	56198	104494	3.59%	0.373%
32	13.269	1897	1900	1907	rVB2	78978	126371	4.35%	0.451%
33	13.880	2001	2004	2014	rVB4	153372	289007	9.94%	1.032%
34	14.033	2024	2030	2042	rBV2	974472	2006095	68.98%	7.165%
35	15.074	2203	2207	2216	rVB	482138	1030670	35.44%	3.681%
36	15.380	2255	2259	2265	rVB	240021	378686	13.02%	1.352%

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BU-02-031125

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.445	2265	2270	2275	rBV	307501	480022	16.50%	1.714%
38	15.510	2276	2281	2284	rBV	401816	645117	22.18%	2.304%
39	16.986	2528	2532	2541	rVB2	179458	377495	12.98%	1.348%
40	17.433	2604	2608	2620	rVB	147185	325479	11.19%	1.162%

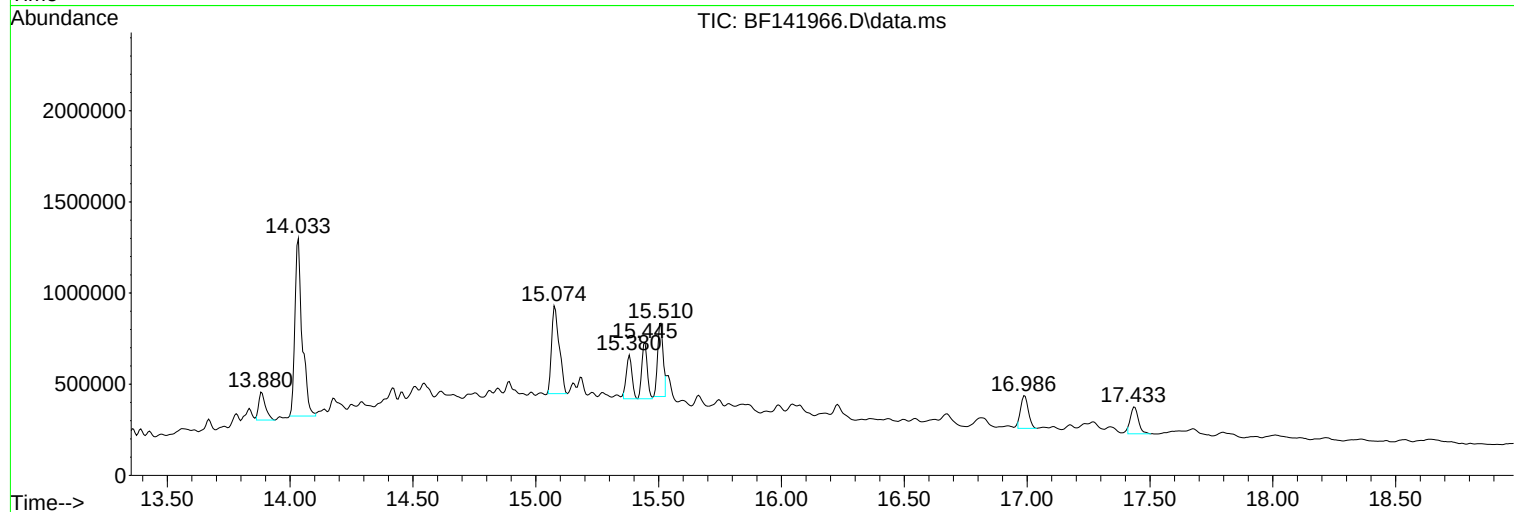
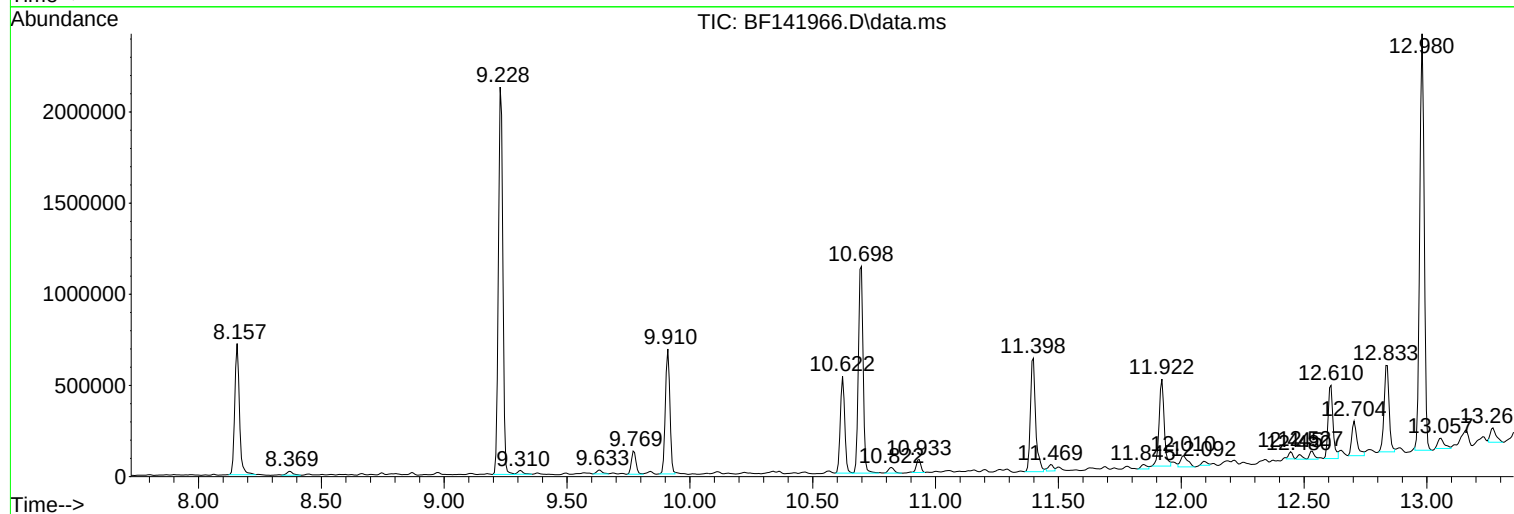
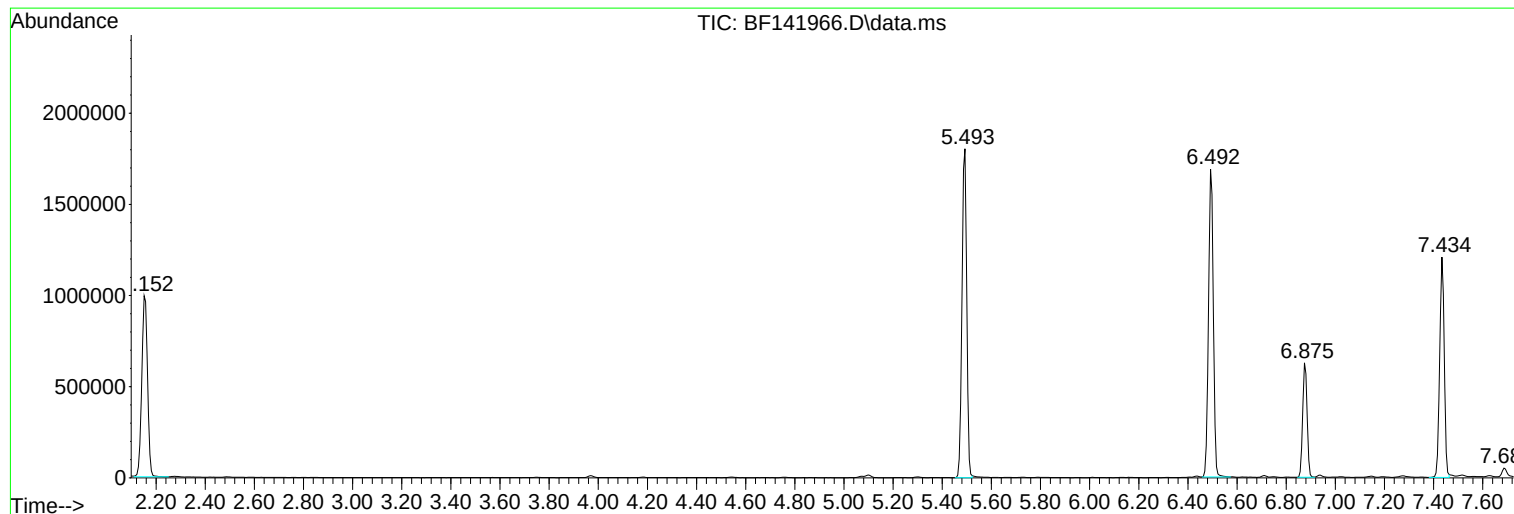
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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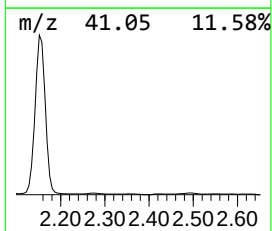
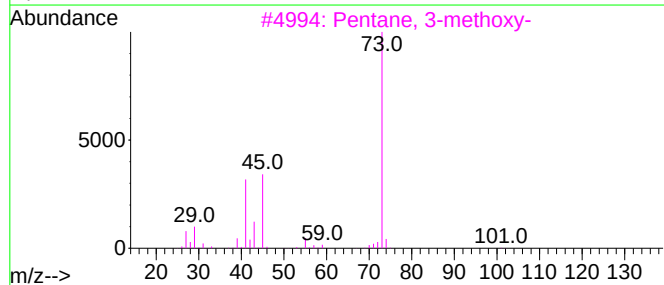
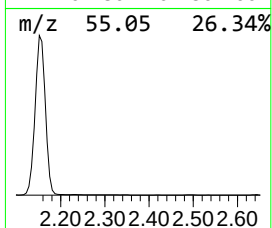
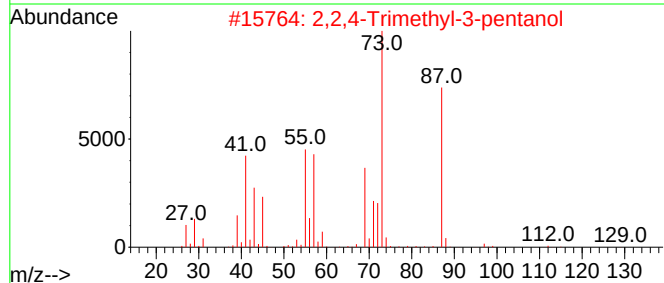
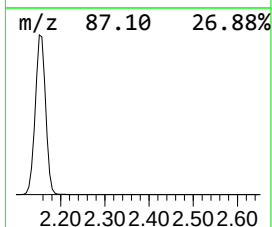
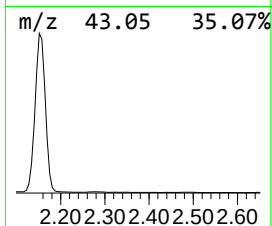
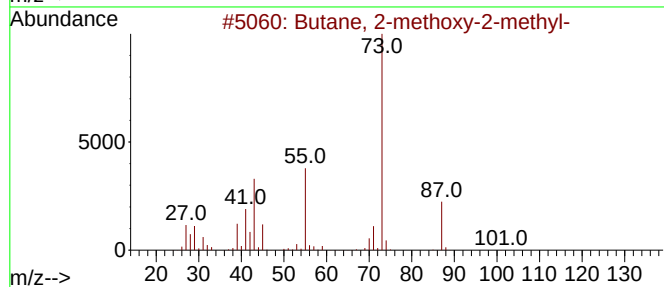
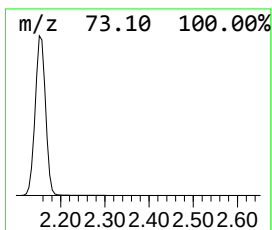
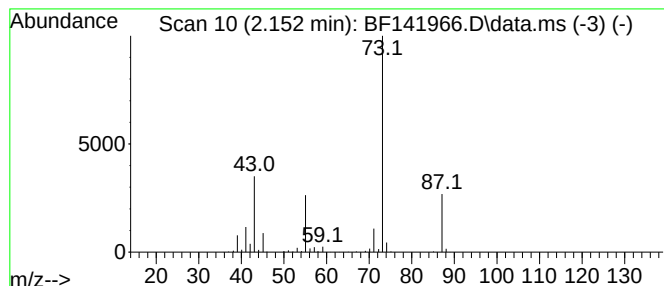
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	41.18 ng	1617330	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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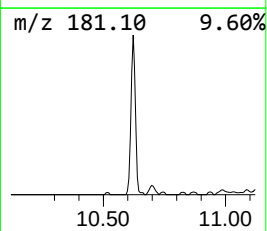
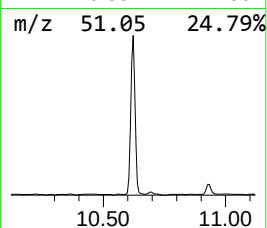
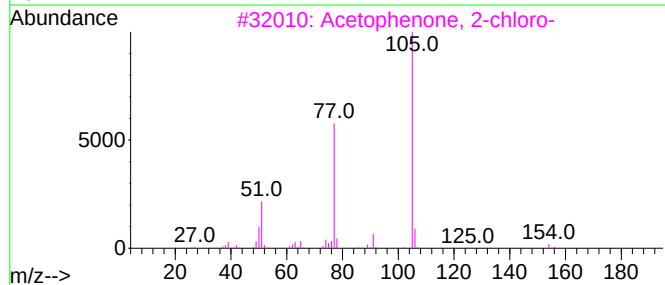
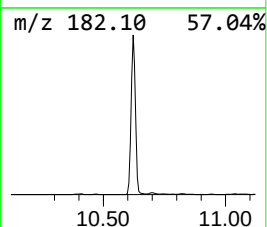
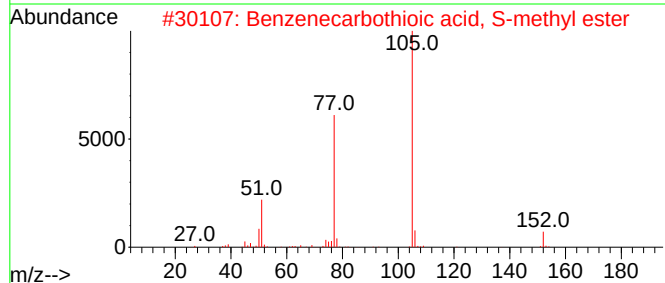
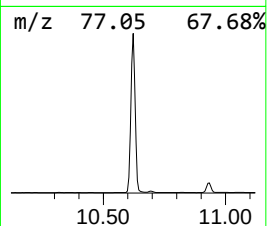
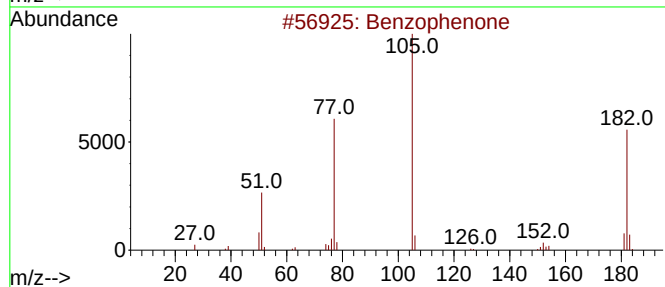
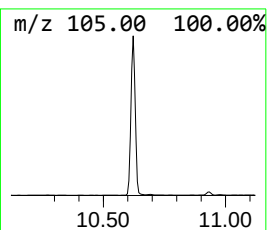
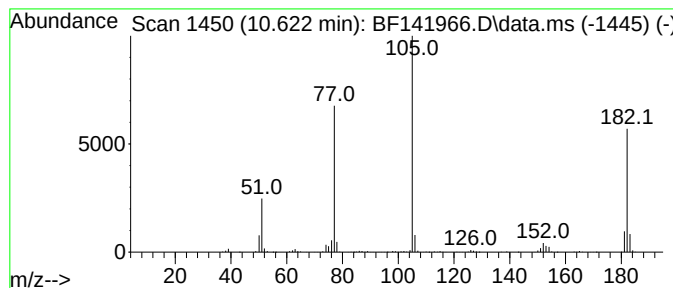
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	15.50 ng	664771	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



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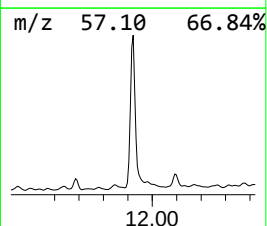
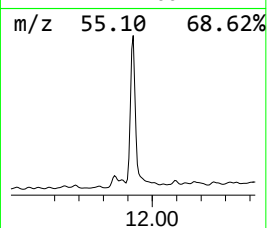
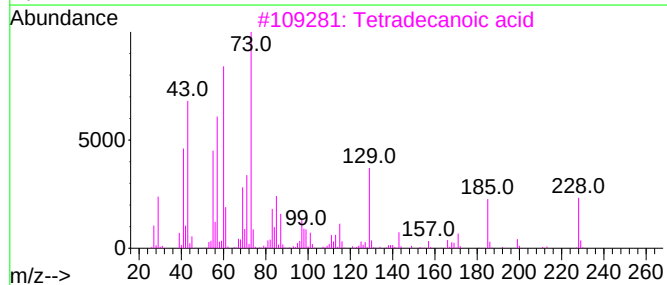
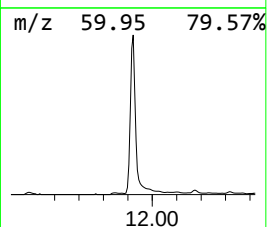
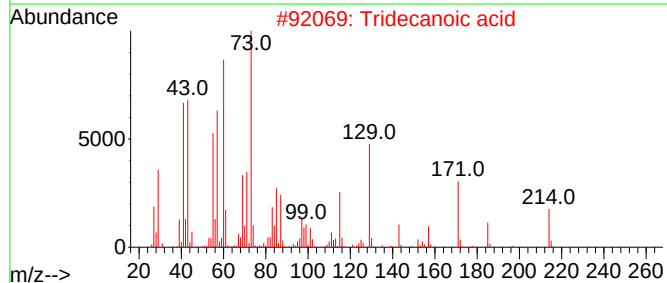
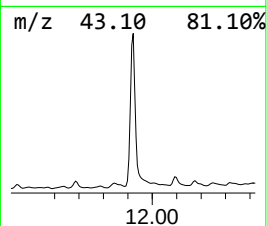
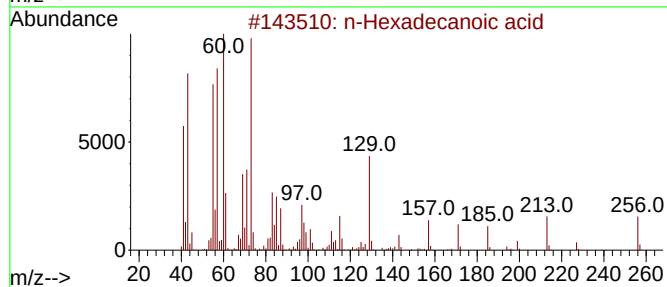
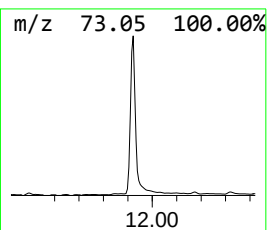
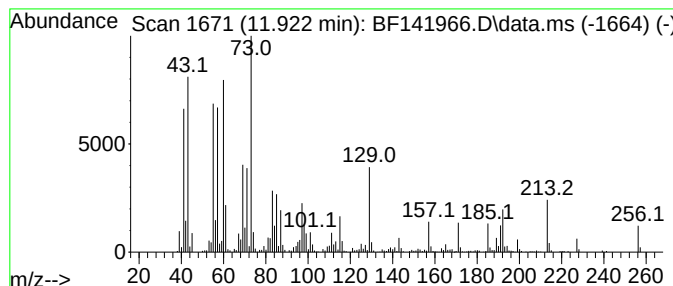
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	14.93 ng	684945	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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ClientSampleId :
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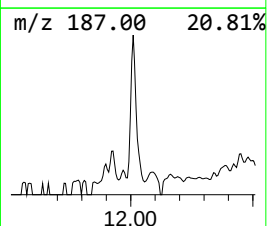
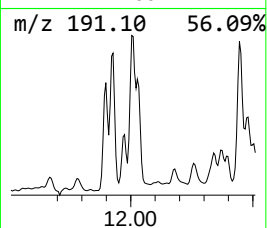
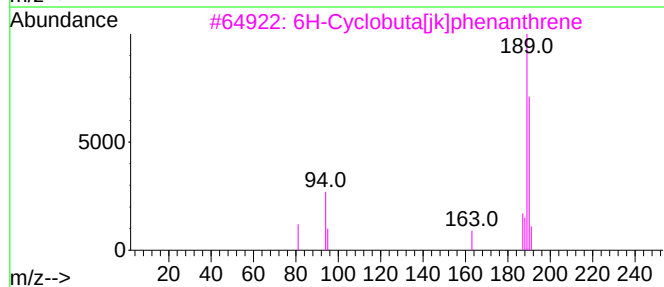
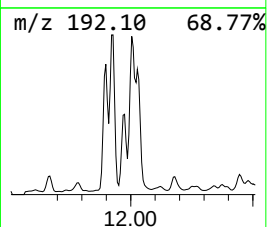
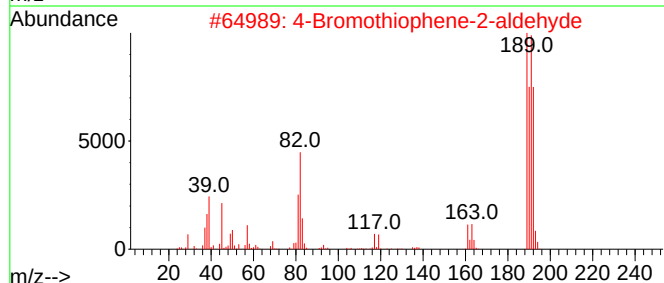
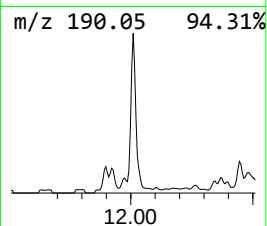
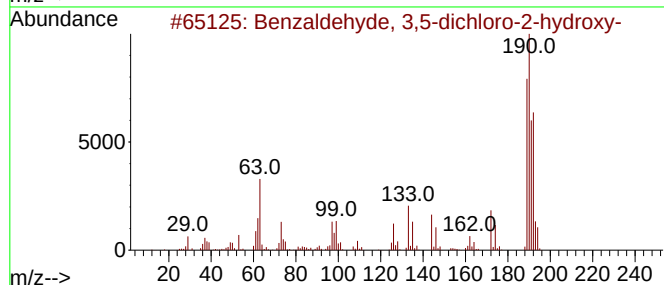
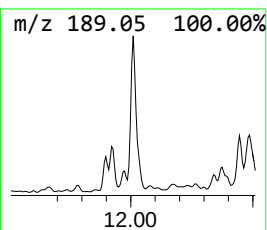
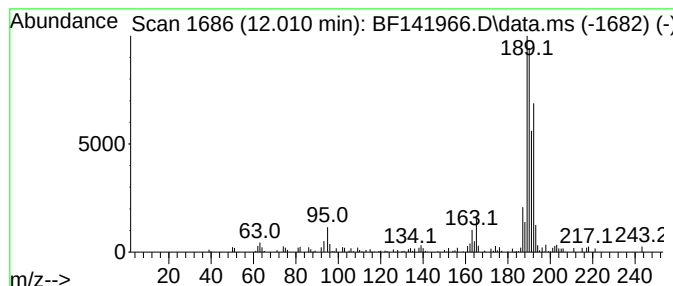
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.71 ng	124232	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	62
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	52
4			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43
5			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43



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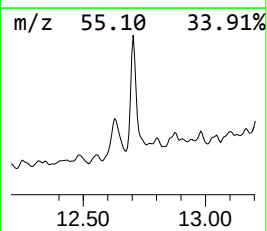
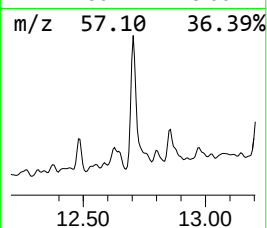
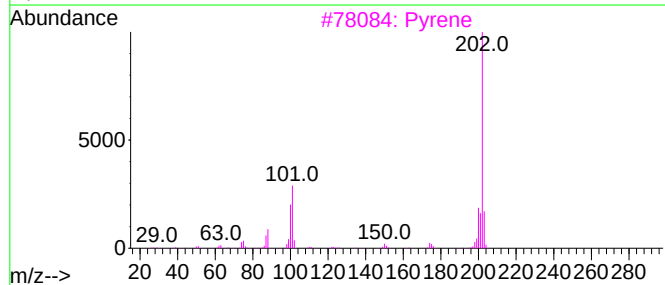
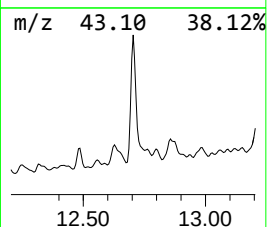
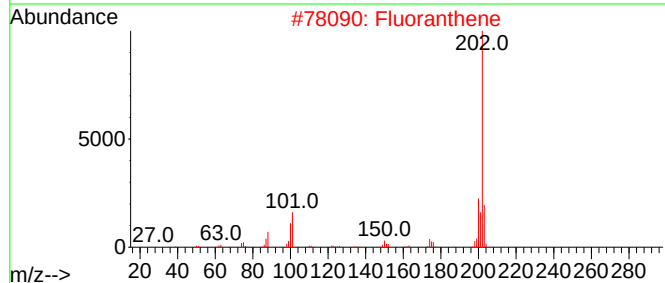
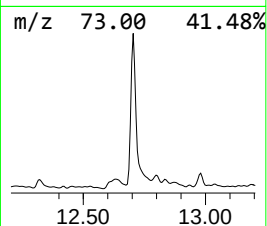
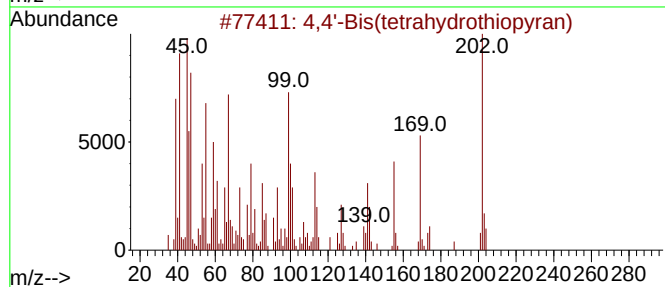
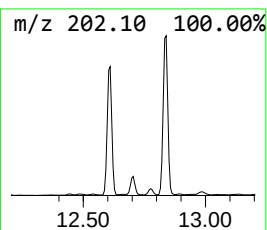
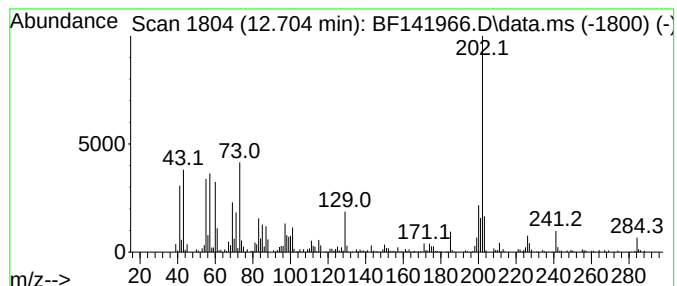
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.16 ng	282562	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	94
2			Fluoranthene	202	C16H10	000206-44-0	70
3			Pyrene	202	C16H10	000129-00-0	55
4			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	53
5			4-Amino-2-methylquinoline-6-carb...	202	C11H10N2O2	099984-73-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141966.D
Acq On : 14 Mar 2025 15:38
Operator : RC/JU
Sample : Q1545-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-031125

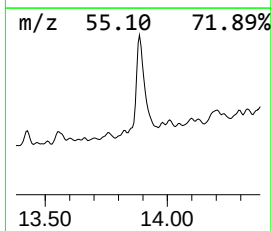
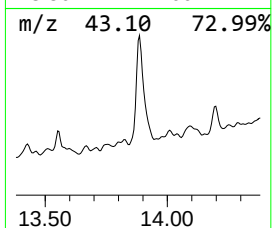
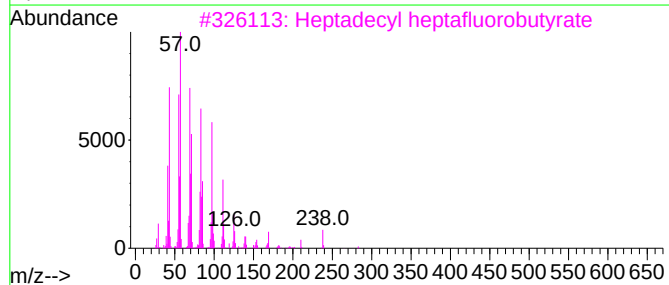
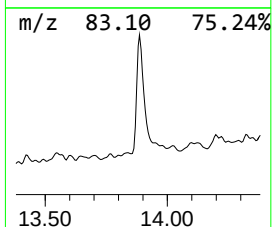
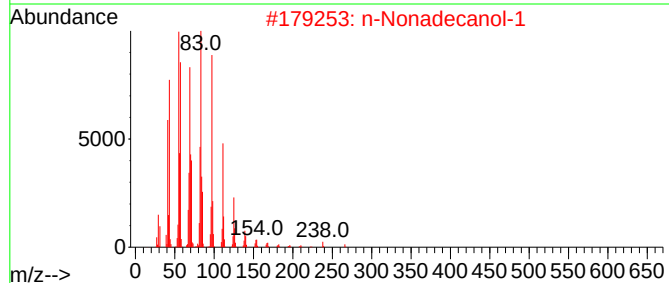
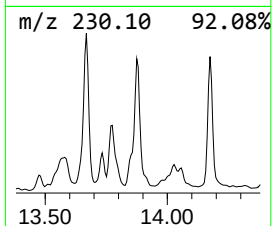
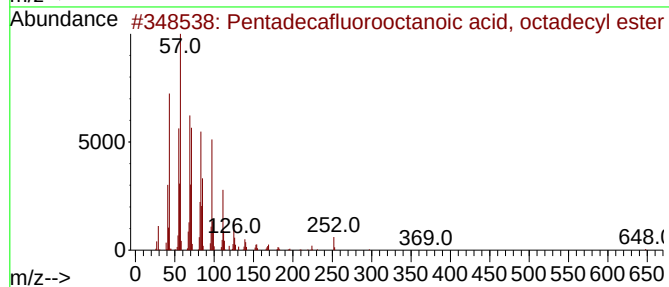
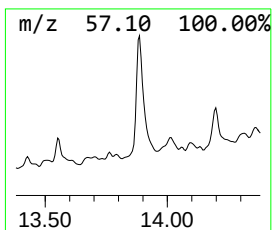
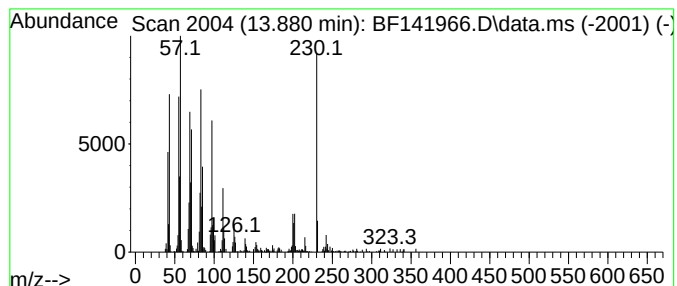
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.88 ng	289007	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86
4			1-Tetracosene	336	C24H48	010192-32-2	80
5			1-Hexacosene	364	C26H52	018835-33-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141966.D
Acq On : 14 Mar 2025 15:38
Operator : RC/JU
Sample : Q1545-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-031125

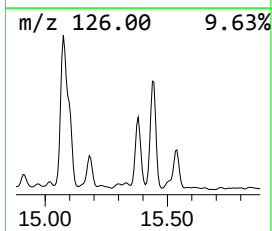
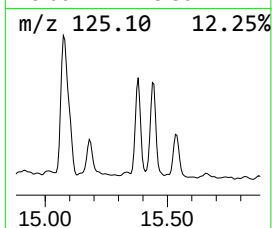
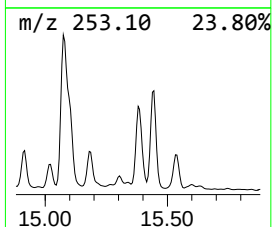
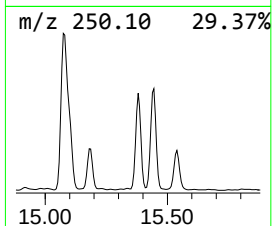
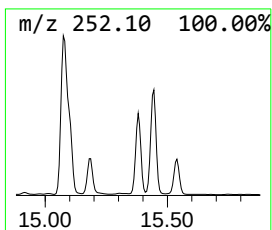
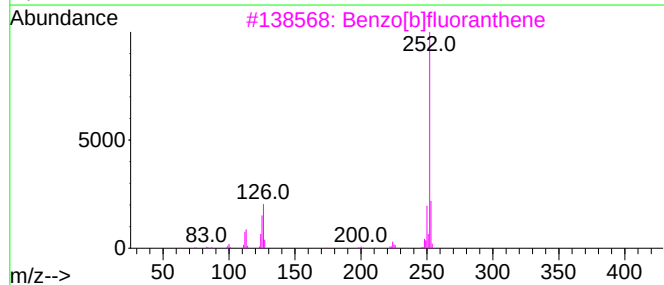
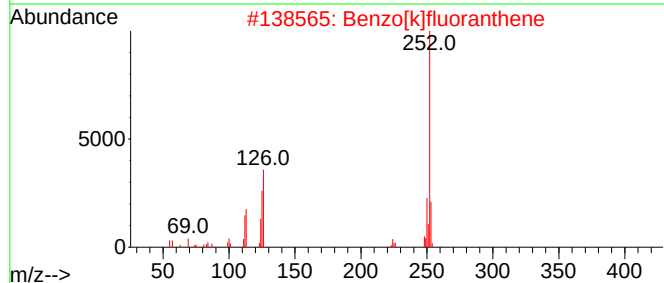
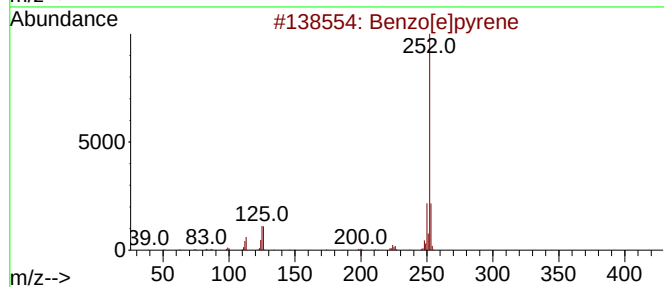
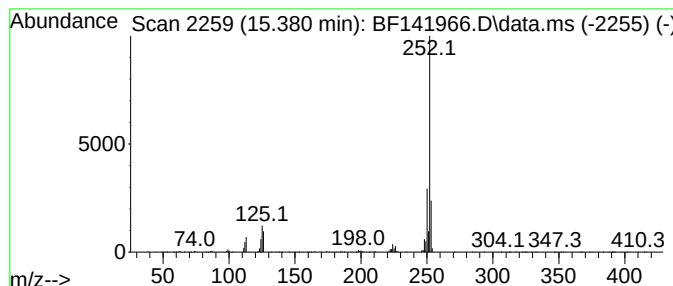
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	11.74 ng	378686	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031425\
Data File : BF141966.D
Acq On : 14 Mar 2025 15:38
Operator : RC/JU
Sample : Q1545-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-031125

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	41.2	ng	1617330	1	6.875	785567	20.0
Benzophenone	10.622	15.5	ng	664771	3	9.910	857523	20.0
n-Hexadecanoic ...	11.922	14.9	ng	684945	4	11.398	917659	20.0
Benzaldehyde, 3...	12.010	2.7	ng	124232	4	11.398	917659	20.0
4,4'-Bis(tetra...	12.704	6.2	ng	282562	4	11.398	917659	20.0
Pentadecafluoro...	13.880	2.9	ng	289007	5	14.033	2006100	20.0
Benzo[e]pyrene	15.380	11.7	ng	378686	6	15.509	645117	20.0